# Exam: Introduction to Condensed Matter Theory

*Thursday, April 6, 2017*

*The total number of points is 50. Do not forget to write your name and the student number on the first sheet. Good luck.*

1. **Displacement and momentum of ions in a crystal:** A crystal with a Bravais lattice is formed by ions of mass $M$. The displacement, $\boldsymbol{Q}_n$, and the momentum, $\boldsymbol{P}_n$, of the $n$-th ion are expressed in terms of the phonon creation and annihilation operators by

$$\begin{cases} \boldsymbol{Q}_n = \frac{1}{\sqrt{N}}\sum_{q\lambda} \boldsymbol{e}_{q\lambda}\sqrt{\frac{\hbar}{2M\omega_{q\lambda}}}\left(b_{q\lambda}e^{i\boldsymbol{q}\cdot\boldsymbol{X}_n^{(0)}} + b^\dagger_{q\lambda}e^{-i\boldsymbol{q}\cdot\boldsymbol{X}_n^{(0)}}\right), \\ \boldsymbol{P}_n = \frac{1}{i\sqrt{N}}\sum_{q\lambda} \boldsymbol{e}_{q\lambda}\sqrt{\frac{\hbar M\omega_{q\lambda}}{2}}\left(b_{q\lambda}e^{i\boldsymbol{q}\cdot\boldsymbol{X}_n^{(0)}} - b^\dagger_{q\lambda}e^{-i\boldsymbol{q}\cdot\boldsymbol{X}_n^{(0)}}\right). \end{cases} \tag{1}$$

Show that the average $\langle \boldsymbol{Q}_n \cdot \boldsymbol{P}_n\rangle$ is independent of temperature and is given by

$$\langle \boldsymbol{Q}_n \cdot \boldsymbol{P}_n\rangle = \frac{3}{2}i\hbar. \tag{2}$$

[10 points]

2. **Elastic energy of a cubic crystal:** Consider a cubic crystal that belongs to the crystal class $2/m\bar{3}$ ($T_h$). Its point group contains the 180°-rotation around the $z$ axis, $2_z = (-x,-y,z)$, the 120°-rotation around the axis along the [111] direction, $3_{[111]} = (z,x,y)$, and inversion, $I = (-x,-y,-z)$.

   (a) Show that the crystal is also invariant under mirror, $m_z = (x,y,-z)$. [2 points]

   (b) Give the most general expression for the harmonic lattice energy of this cubic crystal in terms of the components of the strain tensor, $u_{\alpha\beta}$. [8 points]

3. **Magnons in a square lattice ferromagnet:** Consider a ferromagnet in which spins form a square lattice with the lattice constant $a$. The spin Hamiltonian has the form,

$$\hat{H}_{\text{spin}} = -J\sum_n(\mathbf{S}_n\cdot\mathbf{S}_{n+x} + \mathbf{S}_n\cdot\mathbf{S}_{n+y}) - \mu H\sum_n S^z_n, \tag{3}$$

where $\mathbf{S}_n$ denotes spin at the site $n$ with the coordinate $\boldsymbol{X}_n = (n_x a, n_y a)$ and $\mathbf{S}_{n+x}$/$\mathbf{S}_{n+y}$ is the spin at the neighboring site along the $x$/$y$ axis, e.g. $\boldsymbol{X}_{n+x} = ((n_x+1)a, n_y a)$. The first sum in Eq.(3) is the ferromagnetic exchange interaction between neighboring spins ($J > 0$) and the second term is the Zeeman interaction with the magnetic field $H$ along the $z$ axis.

The Dyson-Maleev transformation,

$$\begin{cases} S_n^- = S_n^x - iS_n^y & = \sqrt{2S}b_n^\dagger, \\ S_n^+ = S_n^x + iS_n^y & = \sqrt{2S}\left(1 - \frac{b_n^\dagger b_n}{2S}\right) b_n, \\ S_n^z = S - b_n^\dagger b_n, \end{cases} \tag{4}$$

expresses the spin operator, $\mathbf{S}_n$, in terms of the annihilation and creation operators of bosons, $b_n$ and $b_n^\dagger$, obeying the commutation relations,

$$[b_n, b_m^\dagger] = \delta_{n,m}, \quad [b_n, b_m] = [b_n^\dagger, b_m^\dagger] = 0. \tag{5}$$

(a) Express the spin Hamiltonian (3) in terms of the Bose operators, assuming that $S \gg 1$ (large spin) and keeping only the terms proportional to $S^2$ and $S^1$.
*Hint: For large spin,* $S_n^+ \approx \sqrt{2S}b_n$. [4 points]

(b) Re-write the boson Hamiltonian in terms of the magnon operators, $b_{\boldsymbol{k}}$ ($b_{\boldsymbol{k}}$ annihilates the spin wave with the wave vector $\boldsymbol{k}$):

$$\begin{cases} b_{\boldsymbol{k}} & = \frac{1}{\sqrt{N}} \sum_n e^{-i\mathbf{k}\boldsymbol{X}_n} b_{n\sigma}, \\ \\ b_{n\sigma} & = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{X}_n} b_{\boldsymbol{k}\sigma}, \end{cases} \tag{6}$$

where $N$ is the total number of lattice sites. [4 points]

(c) Find the dependence of the magnon energy, $\varepsilon_{\boldsymbol{k}}$, on the wave vector $\mathbf{k}$. Explain why the magnon spectrum has no gap in zero magnetic field and why the applied field opens a gap. [2 points]

4. **Electrons in a cubic crystal:** Consider an ideal gas of electrons that can occupy the sites of the cubic lattice with the lattice constant $a$. The tight-binding Hamiltonian describing the hoping of electrons between nearest-neighbor sites has the form,

$$H = -t \sum_{n\sigma} \sum_{\lambda=x,y,z} \left( c_{n\sigma}^\dagger c_{n+\lambda,\sigma} + c_{n+\lambda,\sigma}^\dagger c_{n\sigma} \right), \tag{7}$$

where $c_{n,\sigma}$ is the operator annihilating electron at the site $n$ with the spin projection $\sigma = \uparrow, \downarrow$ and $n + \lambda$ denotes the nearest-neighbor site in the direction $\lambda = x, y, z$ (for example, $\boldsymbol{X}_{n+x} = \boldsymbol{X}_n + a\hat{x}$).

(a) Derive Heisenberg equation of motion for the electron annihilation operator $c_{n\sigma}$. [4 points]

*Hint: Keep in mind that electron operators obey anti-commutation relations.*

(b) Re-write the Hamiltonian (7) in terms of the Bloch wave operators, $c_{k\sigma}$:

$$\begin{cases} c_{k\sigma} = \frac{1}{\sqrt{N}} \sum_n e^{-ikX_n} c_{n\sigma}, \\ \\ c_{n\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{ikX_n} c_{k\sigma}, \end{cases} \tag{8}$$

where $N$ is the total number of lattice sites. [4 points]

(c) Find the energy of electron with the wave vector $k$, $\varepsilon_k$. Find the band width, $W$ (difference between the maximal and minimal electron energies). [2 points]

*Hint: $\varepsilon_k$ can be found directly from the the electron Hamiltonian in the momentum representation or from $i\hbar \frac{\partial c_{k\sigma}}{\partial t} = \varepsilon_k c_{k\sigma}$. Equation of motion for $c_{k\sigma}$ can be obtained by Fourier transformation of the equation for $c_{n\sigma}$.*

5. **Kramers-Kronig relations, plasmon and sum rule**

(a) The real and imaginary parts of the dielectric susceptibility, $\chi'(\omega)$ and $\chi''(\omega)$, satisfy

$$\chi'(\omega) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} d\xi \frac{\chi''(\xi)}{\xi - \omega}, \tag{9}$$

where $P\int$ is the principal value integral. What is the physical origin of this relation? [2 points]

(b) Prove that the Kramers-Kronig relation (9) can be re-written as the principle value integral over positive frequencies:

$$\chi'(\omega) = \frac{2}{\pi} P \int_{0}^{+\infty} d\xi \frac{\xi \chi''(\xi)}{\xi^2 - \omega^2}. \tag{10}$$

[2 points]

*Hint: Use a relation between $\chi''(-\omega)$ and $\chi''(\omega)$.*

(c) Show that the imaginary part of the dielectric susceptibility of metal, $\chi''(\omega)$, obeys the sum rule,

$$\int_0^{\infty} d\omega \omega \chi''(\omega) = \frac{\omega_p^2}{8},$$

where $\omega_p$ is the plasmon frequency. [6 points]

*Hint: Use the relation* $\varepsilon(\omega) = 1 + 4\pi\chi(\omega)$ *between the dielectric function,* $\varepsilon(\omega)$, *and the dielectric susceptibility,* $\chi(\omega)$. *Use the asymptotic form of* $\varepsilon(\omega)$ *at high-frequencies.*